Symmetry and quantum transport on networks

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Abstract

We study the classical and quantum transport processes on some finite networks and model them by continuous-time random walks (CTRW) and continuous-time quantum walks (CTQW), respectively. We calculate the classical and quantum transition probabilities between two nodes of the network. We numerically show that there is a high probability to find the walker at the initial node for CTQWs on the underlying networks due to the interference phenomenon, even for long times. To get global information (independent of the starting node) about the transport efficiency, we average the return probability over all nodes of the network. We apply the decay rate and the asymptotic value of the average of the return probability to evaluate the transport efficiency. Our numerical results prove that the existence of the symmetry in the underlying networks makes quantum transport be less efficient than the classical one. In addition, we find that the increasing of the symmetry of these networks decreases the efficiency of quantum transport on them.

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1 Introduction

Quantum walk(QW) as a generalization of random walk(RW) is obtained by endowing the walker with quantum properties [1, 2]. The QW has been largely based on two standard variants, the discrete time QW(DTQW) [3] and the continuous-time QW(CTQW) [1]. In recent years, the DTQWs have been investigated on trees [4], random environment [5], single and entangled particles [6, 7, 8]. The CTQWs have been studied on line [9, 10, 11, 12], cycle [13, 14], one-dimension regular network [15], regular graphs [16], odd graphs [17], cayley tree [18, 19, 20], hypercube [21], small-world network [22], star graphs [23, 24], dendrimer [25], restricted geometries [26], Apollonian network [27] and one-dimensional and two-dimensional networks with periodic boundary conditions [28, 29]. Moreover, the decoherent QWs have been considered on hypercube [30], cycle [31, 32], long-range interacting cycle [33, 34] and one-dimension regular network [35].

Since the QWs may exploit quantum mechanical effects such as entanglement and interference, the only special experimental techniques can be candidate to implement them. Recently, some experimental implementations of both QW variants have been reported e.g. on microwave cavities [36], ground state atoms [37], the orbital angular momentum of photons [38], waveguide arrays [39] or Rydberg atoms [40, 41].

Since RWs generate the classical algorithms in computer science and model the diffusion phenomena and non-deterministic motion on the complex networks [42], it can be expected that their quantum extensions(QWs) provide tool to implement quantum computing and to model quantum processes [43]. In quantum computing, it is a primary goal to determine when quantum computers can solve problems faster than classical computers [44, 45]. Grover in 1996 proved that a classical computer requires $\mathcal{O}(N)$ steps to finding marked item among N items, whereas quantum computer can solve it using only $\mathcal{O}(\sqrt{N})$ steps [46]. Several implementations to Grover's algorithm have been reported by CTQW [1, 47, 48] and DTQW [49, 50, 51]. To implement Grover's algorithm, the all items must be accessible by local moves. For instance, if items are located on the one-dimensional line, traveling from one end of the line to the other end requires N moves, thus the classical or quantum algorithms can not find a marked item in less time than $\mathcal{O}(N)$ [47]. It is interesting to consider a one-dimensional line and then gradually to change its structure so that, in every step, items on it to be accessible by the lesser moves, as shown in Figs. 1(a-e).
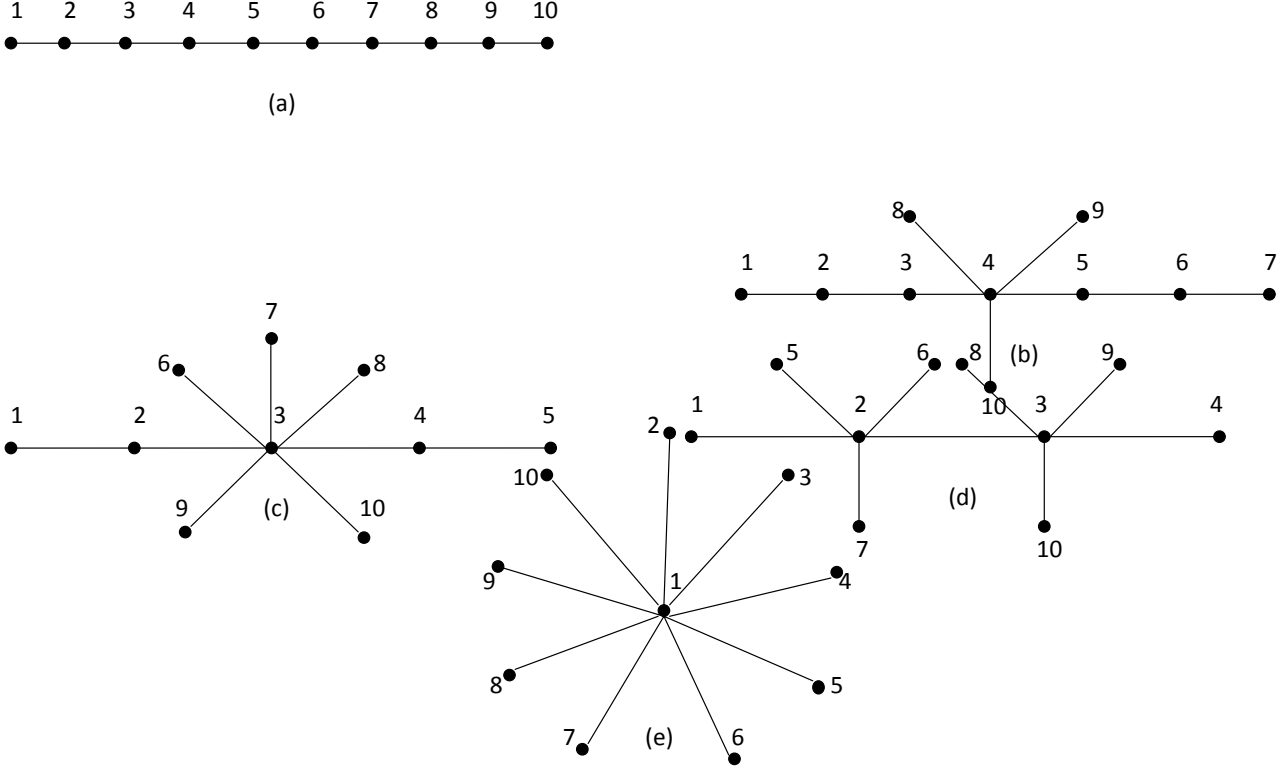
Figure 1: Figs. 1(a)-(e) show some networks with ten nodes and nine edges.

On the other hand, in recent years the complex networks have been applied to model very diverse systems in nature such as lattices in solid state physics and condensed matter [52, 53, 54, 55]. In this modeling process, the components of system and interactions among them are considered as nodes and bonds of network, respectively. It is difficult to study the complex networks having many nodes or bonds or both. But the most complex networks are constructed from simpler networks which the number of nodes and the number of bonds are smaller. Since these simpler networks can successfully explain some features of whole network, there is an upsurge of interest in

studying of their various aspects. Hence, by studying of RW and QW on the above mentioned simple networks, we also highlight the interplay between the diffusion process and the network symmetry.

In this paper, we first calculate transition probabilities between two nodes of network for the CTRWs and CTQWs, then we numerically show that for CTQWs on the mentioned networks due to interference phenomenon, even for long times, there is high probability to find the walker at the initial node. Thus, the quantum transition probability distribution on underlying networks depends significantly on the initial node. To get a global information about efficiency of walk, we average the return probability over all nodes of network. Then, we evaluate the transport efficiency on networks(a-e) by the rate decay and by the asymptotic value of average return probability. The numerical results show that the existence of symmetry in the mentioned networks causes the quantum transport to be less efficient than the classical counterpart. In other words, the results denote that the increasing of the symmetry of these networks decreases the efficiency of quantum transport on them.

Our paper is structured as follows: after a brief summary of the main concepts and of the formulae concerning CTQWs in Sec. 2, we study the quantum transition probabilities and their long time average on the mentioned networks, in Sec. 3. In Sec. 4, we especially focus on the average return probabilities and the efficiency of classical and quantum walks. Finally, in Sec. 5 the conclusions are presented.

2   CTQWs on networks

In general, every network can be characterized by a graph G that consists of a finite nonempty set V of N vertices together with a prescribed set X of q unordered pairs of distinct vertices of V so that each pair $x = \{u, v\}$ of vertices in X is a edge of G [56].

Algebraically, a graph can be described by its adjacency matrix A whose elements are $A(i, j) = 1$ for $(i, j) \in X$ and $A(i, j) = 0$ otherwise. The Laplacian operator is then defined as $L = Z - A$, where Z is a diagonal matrix and $Z_{j,j}$ is the degree of vertex j. Classically, the evolution of CTRW is governed by the following master equation [57]:

$$\frac{d}{dt}P_{k,j} = \sum_{l=1}^{N} T_{kl}P_{l,j},$$

(1)

where $P_{k,j}(t)$ is the conditional probability to find the walker at time t at node k when starting at node j.

The matrix T is the transfer matrix of the walk, $T = (T_{kj})$, and relates to the Laplace matrix through $T = -\gamma L$, where we assume an unbiased CTRW so that the transmission rates of all bonds are equal and set $\gamma \equiv 1$.

The CTQW as the quantum mechanical extension of CTRW is obtained by replacing the Hamiltonian of the system by the classical transfer matrix, $H = -T$ [1].

We denote the state associated with node j of network as $|j\rangle$ and take the set $\{|j\rangle\}$ to be orthonormal. Thus, the solution of Eq. (1) is

$$P_{k,j}(t) = \langle k|e^{tT}|j\rangle. \tag{2}$$

Quantum mechanically, the states $|j\rangle$ span the whole accessible Hilbert space. The time evolution of state $|j\rangle$ starting at time t_0 is given by $|j,t\rangle = U(t,t_0)|j\rangle$, where $U(t,t_0) = \exp[-iH(t-t_0)]$ is the quantum mechanical evolution operator. Hence, transition amplitude $\alpha_{k,j}(t)$ from state $|j\rangle$ at the time 0 to state $|k\rangle$ at time t is

$$\alpha_{k,j}(t) = \langle k|e^{-iHt}|j\rangle. \tag{3}$$

From the Schrodinger Equation(SE), we obtain

$$i\frac{d}{dt}\alpha_{k,j}(t) = \sum_{l=1}^{N} H_{kl}\alpha_{l,j}(t), \tag{4}$$

where $\hbar = 1$. We assume that E_n and $|q_n\rangle$ denote the nth eigenvalue and eigenvector of H, respectively. The classical and quantum transition probabilities between two nodes can be written as [58],

$$P_{k,j}(t) = \sum_{n=1}^{N} e^{-tE_n}\langle k|q_n\rangle\langle q_n|j\rangle \tag{5}$$

$$\pi_{k,j}(t) = |\alpha_{k,j}(t)|^2 = |\sum_{n=1}^{N} e^{-itE_n}\langle k|q_n\rangle\langle q_n|j\rangle|^2. \tag{6}$$

Note that the normalization condition for $P_{k,j}(t)$ is $\sum_{k=1}^{N} P_{k,j}(t) = 1$ and for $\alpha_{k,j}(t)$ is $\sum_{k=1}^{N} |\alpha_{k,j}(t)|^2 = 1$.

Classically, the transition probabilities converge to the equip-partitioned

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probability $\frac{1}{N}$, whereas the quantum probabilities do not reach any finite value but after some time fluctuate about a constant value. This value is determined by the long time average(LTA) which is defined by using Eq. (6) [29]:

$$\chi_{k,j} = \lim_{T \longrightarrow \infty} \frac{1}{T} \int_0^T \pi_{k,j}(t)dt = \sum_{n,m} \delta_{E_n,E_m} \langle k|q_n \rangle \langle q_n|j \rangle \langle j|q_m \rangle \langle q_m|k \rangle, \qquad (7)$$

where $\delta_{E_n,E_m} = 1$ for $E_n = E_m$ and $\delta_{E_n,E_m} = 0$ otherwise. Since some eigenvalues of H may be degenerate, the sum in the Eq. (7) contains terms belonging to different eigenvectors.

3   Quantum transition probabilities

In this section, we illustrate the importance of choosing the initial node in CTQWs process on the networks. For this aim, we first consider the quantum transition probabilities in intermediate times when the walker started from a special node. Then, we generalize our result for long times and the whole nodes by studying the LTA probabilities.

To obtain the quantum transition probabilities(see Eq. (6)), we need all the eigenvalues and eigenvectors of H, thus we make use of standard software MATLAB.

In Fig. 2(a-e) we present the quantum transition probabilities $\pi_{k,j}(t)$ for networks(a-e) where $j = 5, 4, ..., 1$, respectively. Figs. 2(a-e) show the high values for $\pi_{5,5}$, $\pi_{4,4}$, $\pi_{3,3}$, $\pi_{2,2}$ and $\pi_{1,1}$. In other words, these figures prove that at short times(from $t = 1s$ to $t = 20s$), the quantum return probability is large and thus the CTQWs hold such dependence significantly on given starting node.

Now it is natural to pose the following questions:

Whether the such behavior continues at long times?

Do the CTQWs hold such dependence on the other starting nodes?

To address these questions, in Figs. 3(a-e) we plotted the LTA probabilities for all nodes k and j pertaining to networks(a-e), respectively.

The axes x and y show nodes k and j of network respectively, and $\chi_{k,j}$ is presented on the axis z. Figs. 3(a-e) show the symmetry characterizing the quantum transition probability, namely $\chi_{k,j} = \chi_{j,k}$. This can be derived directly from Eq. (7), recalling that H itself is symmetric and real.
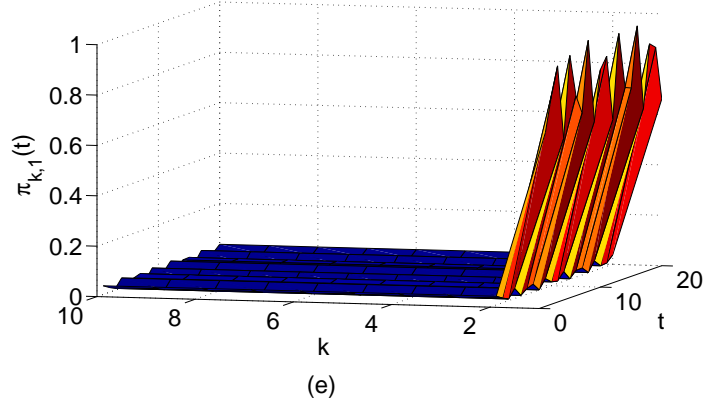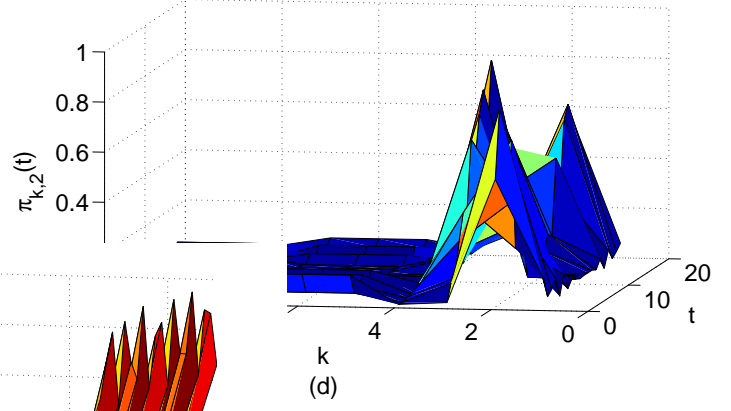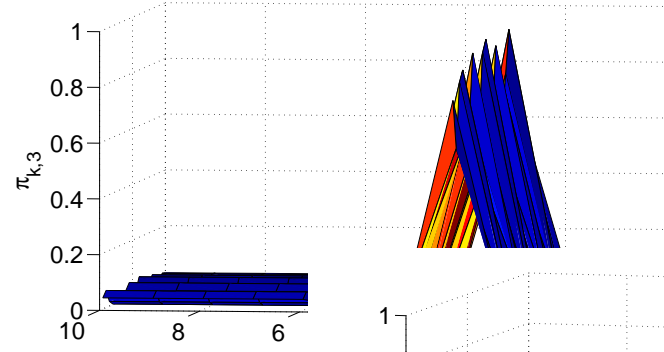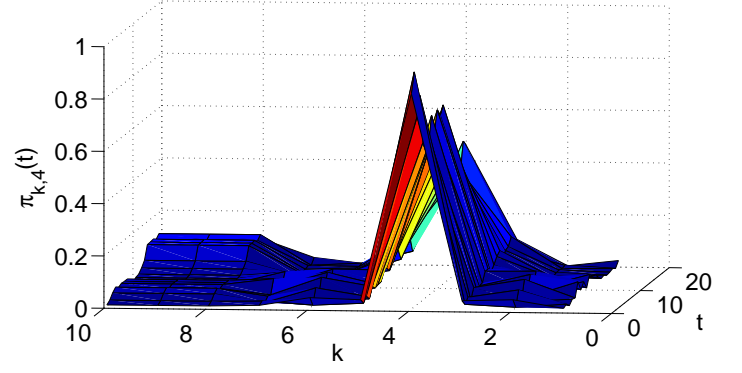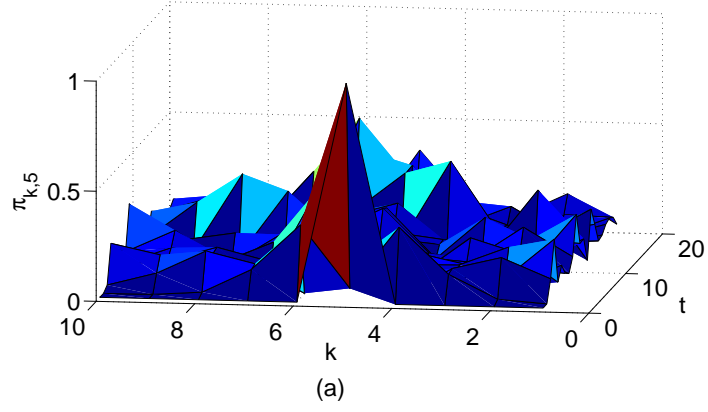
(a)

(b)

(c)

(d)

(e)

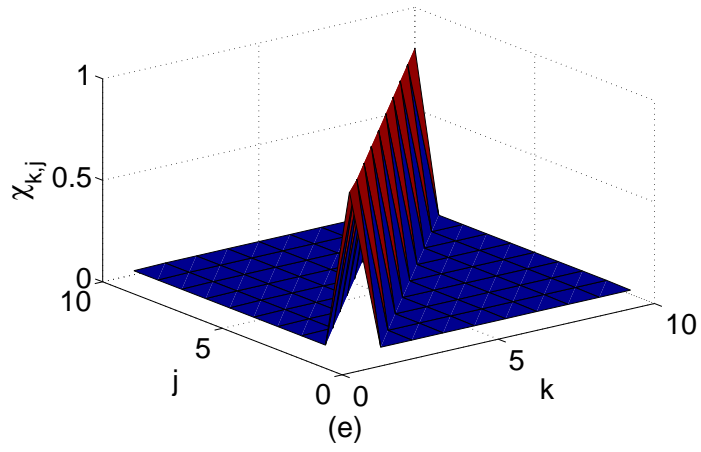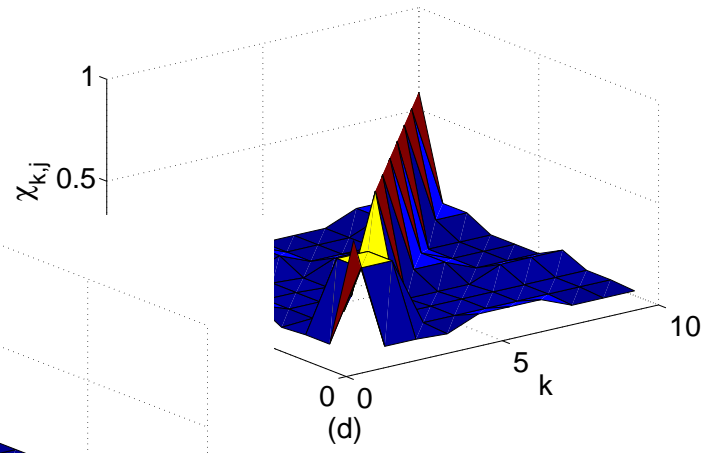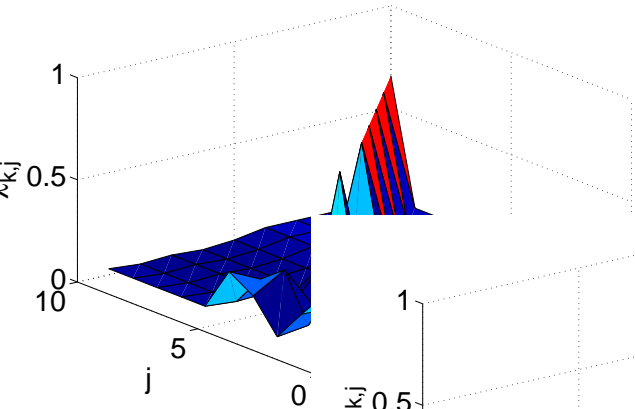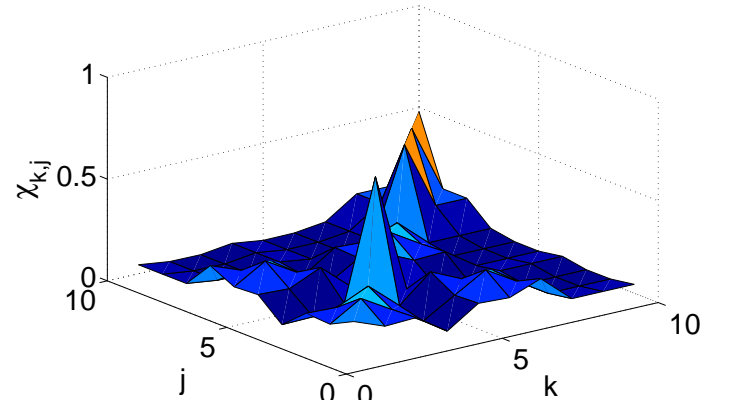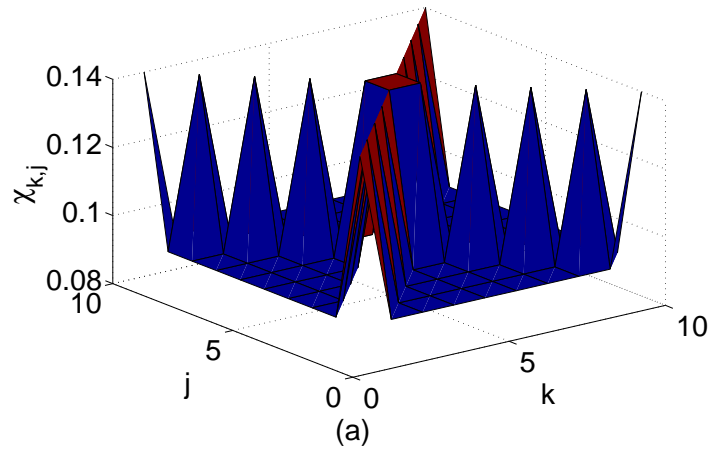Figure 2: Figs. 2(a-e) show the quantum transition probabilities on networks(a-e).

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Figure 3: Figs. 3(a-e) show limiting time average of quantum transition probabilities for networks(a-e).

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In Figs. 3(a-e), $\chi_{5,5}, \chi_{4,4}, \chi_{3,3}, \chi_{2,2}$ and $\chi_{1,1}$ have the high peaks, respectively. These peaks are a consequence of the constructive interference due to reflections at peripheral sites and boundaries. They prove that, even at long times, the quantum probabilities depend on significantly to the starting node which is consistent with findings reported in [20, 29, 25] for Cayley tree(CT) and square torus(ST). Hence, to get global information(independent of the initial node) about CTQWs on networks(a-e), we must average over the whole network nodes.

4   Efficiency of classical and quantum walks

The transport processes implemented by CTRWs and CTQWs will be more efficient if the walker rapidly spreads over the network i.e. there exists a fast delocalization [26]. On the other hand, a fast delocalization implies a small probability to return(or stay) at the initial node, thus the return probability can be good candidate to evaluation the transport efficiency. But according the result of Sec. 3, to get a global information about the transport efficiency, we need a global quantity which is independent of the initial node. For this aim, we average the return probability over all nodes of network and obtain the average return probability.
Hence, the classical and quantum average return probabilities are calculated by the following simple expressions, respectively [58]

$$\bar{P}(t) = \frac{1}{N} \sum_{j=1}^{N} P_{j,j}(t) = \frac{1}{N} \sum_{n=1}^{N} e^{-E_n t} \qquad (8)$$

$$\bar{\pi}(t) = \frac{1}{N} \sum_{j=1}^{N} \pi_{j,j}(t) = \frac{1}{N} \sum_{m,n,j=1}^{N} e^{-i(E_n - E_m)t} |\langle j|q_n\rangle|^2 |\langle j|q_m\rangle|^2 \qquad (9)$$

It is evident that $\bar{P}(t)$ depends only on the eigenvalues and not to the eigenvectors of T while $\bar{\pi}(t)$ depends on both the eigenvalues and the eigenvectors of H. In the quantum case, we can define a lower bound for $\bar{\pi}(t)$ which depends only on the E_n, i.e,:

$$\bar{\pi}(t) \geq | \bar{\alpha}(t) |^2 = | \frac{1}{N} \sum_{n=1}^{N} e^{-iE_n t} |^2 \qquad (10)$$

where $\bar{\alpha}(t) = \frac{1}{N} \sum_{j=1}^{N} \alpha_{j,j}(t)$.
For the CTQW on a simple network with periodic boundary conditions, the

quantum average return probability equals to its lower bound i.e. $\bar{\pi}(t) = |\bar{\alpha}(t)|^2$. The problem of the CTQW on hypercube lattices in higher d-dimensional spaces separates in every direction, thus we have $\alpha_{j,j}^{(d)} = [\alpha_{j,j}(t)]^d$ which results in $\bar{\pi}(t) = |\bar{\alpha}(t)|^2$, too [59].

We denote the degeneracy of eigenvalue E_n by D_n and rewrite Eqs. (8), (10) as

$$\bar{P}(t) = \frac{1}{N} \sum_{E_n} D_n e^{-E_n t} \tag{11}$$

$$\bar{\pi}(t) \geq |\bar{\alpha}(t)|^2 = \frac{1}{N^2} \sum_{E_n, E_m} D_n D_m e^{-i(E_n - E_m)t}. \tag{12}$$

According to Sec. 2, finally $\bar{\pi}(t)$ fluctuates about a stationary(asymptotic) value given by $\bar{\chi}$:

$$\bar{\chi} = \lim_{T \to \infty} \frac{1}{T} \int_0^T \bar{\pi}(t)dt = \frac{1}{N} \sum_{n,m,j} \delta_{E_n, E_m} |\langle j|q_n\rangle|^2 |\langle j|q_m\rangle|^2. \tag{13}$$

By Cauchy-Schwarz inequality or by taking the LTA of $|\bar{\alpha}(t)|^2$, we can obtain a lower bound of $\bar{\chi}$ which does not depend on the eigenvectors [60]:

$$\bar{\chi}_{lb} = \frac{1}{N^2} \sum_{n,m} \delta_{E_n, E_m}. \tag{14}$$

In fact this equation provides the exact asymptotic value of $|\bar{\alpha}(t)|^2$ and the lower bound of asymptotic value of $\bar{\pi}(t)$. Since some eigenvalues of H might be degenerate, the above sum is equal to the number of non-degenerate eigenvalues plus the number squared of degenerate eigenvalues.

The relation among the average return probability and the efficiency of transport can be considered from two different points of view. From the first point of view, the decay rate of the average return probability is proportional to the transport efficiency. The reason being that a quick decrease of the average return probability results -on average- in a quick increase of the probability for the walker to be at any other but the initial node, which provides a more efficient transport. From the second point of view, the asymptotic value of the average return probability has a inverse relation with the transport efficiency, because a large asymptotic value of the average

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return probability implies a large probability to return at the initial node, which means inefficiency.

In [60], authors studied the decay rate of $\bar{P}(t)$ and $|\bar{\alpha}(t)|^2$ on the networks with two distinct eigenvalue spectrums: uniform degeneracy and one highly degeneracy.

They numerically show that for the large networks($N \gg 1$) whose eigenvalues have uniform degeneracy, the quantum walk can be more efficient than the classical one. Also, for the networks whose only eigenvalue E_l has high degeneracy D_l, they used the following approximate equation

$$|\bar{\alpha}(t)|^2 \approx \frac{1}{N^2}[D_l^2 + 2 \sum_{E_n \neq E_l} D_n D_l \cos((E_n - E_l)t)]. \qquad (15)$$

By this equation, they found that $|\bar{\alpha}(t)|^2$ does not show a decay to values fluctuating about $1/N$ but rather to values fluctuating about $1 - 1/N$, thus the quantum transport is less efficient.

In the following, we study the classical and quantum efficiency on the small networks(with few nodes) mentioned in Figs. 1(a-e). Note that all networks(a-e) consist of 10 nodes and 9 links. The symmetry of network is given by whose nodes having the similar situations. For example, nodes 8,9,10 in network(b) and nodes 5,6,7,8,9,10 in network(d) have the similar situations, thus network(d) is symmetrically higher than network(b). On the other hand, the numerical determination of the eigenvalues of networks(a-e) indicates that network(a) has no degenerate eigenvalue while networks(b-e) have one degenerate eigenvalue 1 with the order of degeneracy 2, 4, 6 and 8, respectively. Hence, in networks(a-e) the increasing of network symmetry results in the increasing of degeneracy of eigenvalue 1. We denote the degeneracy of eigenvalue 1 by D_l and represent it as the degree of network symmetry. We divide the problem into two separate cases as follows:

4.1   non-degenerate eigenvalues

Here, we consider network(a) with non-degenerate eigenvalue spectrums. For this network, Eq. (12) can be written as

$$|\bar{\alpha}(t)|^2 = \frac{1}{N^2} \sum_{E_n, E_m} e^{-i(E_n - E_m)t}.$$

From the above equation, one can infer that after long time the only terms with $E_n = E_m$ contribute to the sum and therefore, the equation

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becomes of order $O(\frac{1}{N})$.

Fig. 4(a) shows the temporal behavior of $\bar{P}(t)$, $\bar{\pi}(t)$ and $|\bar{\alpha}(t)|^2$ for network(a). We can see that the classical curve(blue line) does not show the constant value at the intermediate times whereas after $t \approx N = 10s$, not only $|\bar{\alpha}(t)|^2$(solid red line) but also $\bar{\pi}(t)$(green line) fluctuate about the equipartition value $1/10$. As mentioned above, the exact asymptotic value of $|\bar{\alpha}(t)|^2$ and the asymptotic value of $\bar{\pi}(t)$ can be reproduced by Eq. (14). Since the eigenvalue spectrum of network(a) has no degenerate eigenvalue, the only the number of non-degenerate eigenvalues contributes in Eq. (14), resulting in the value $1/10$. To determine the scaling behavior of $\bar{P}(t)$ and $|\bar{\alpha}(t)|^2$, we use the dashed block($t^{-1/2}$) and red(t^{-1}) lines, respectively. These lines show that the quantum return probability decreases faster than classical one, thus the quantum walk is more efficient than the classical random walk.

4.2 degenerate eigenvalues

In the following, we consider the transport efficiency on networks(b-e) with degenerate eigenvalue spectrums. Figs. 4(b-e) represent the temporal behavior of $\bar{P}(t)$, $|\bar{\alpha}(t)|^2$ and $\bar{\pi}(t)$ for networks (b-e), respectively.

In all the figures, for all times, one can see that the quantum average return probability(green curve) is higher than the corresponding classical probability(blue curve), and thus the quantum transport is less efficient than the classical one.

On the other hand, from Figs. 4(b-e), we find that after some time the strong maxima of $\bar{\pi}(t)$ on highly symmetry networks(d,e) can well be reproduced by the lower bound $|\bar{\alpha}(t)|^2$. Also, the increasing of symmetry causes the dashed block curve of Eq. (15), which is plotted for $E_l = 1$, to become very close to the full expression for $|\bar{\alpha}(t)|^2$. For instance, in Fig. 4(e) the positions of the exact curve of $|\bar{\alpha}(t)|^2$ and its approximate equation almost coincide. It means that the only highly degenerate eigenvalues contribute to $|\bar{\alpha}(t)|^2$, and there are only slight deviations due to the remaining ones. Therefore, for highly symmetrical networks(d,e), we can well apply Eq. (15) which proves that, always, $|\bar{\alpha}(t)|^2$ fluctuate about $1 - 1/N$ which is larger than the classical equipartition $1/N$. Thus, the classical transport is more efficient than the quantum one which is in agreement with the above result.
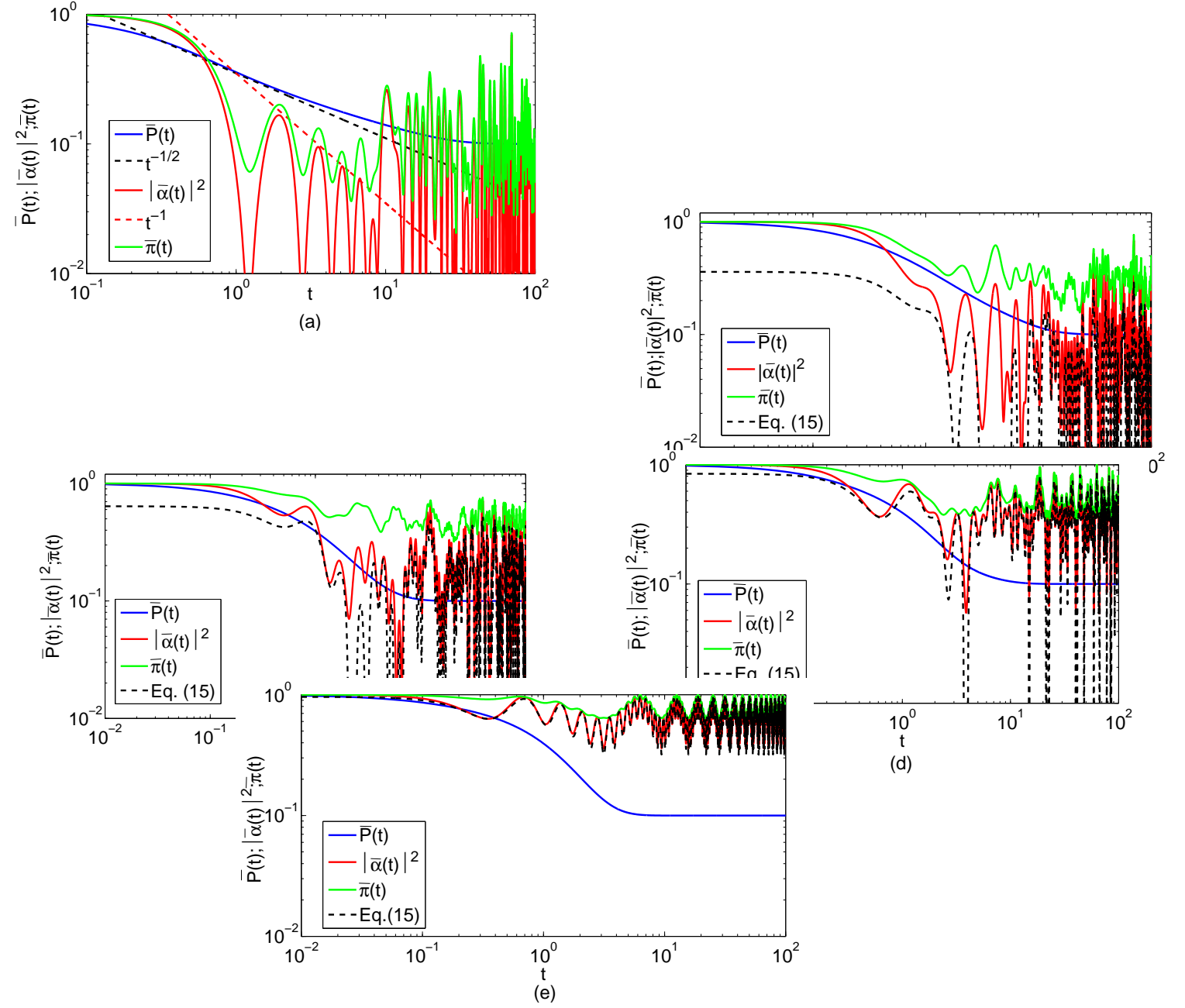
Figure 4: Figs. 4(a-e) show $\bar{P}(t)$, $\bar{\pi}(t)$, $|\bar{\alpha}(t)|^2$ and its approximate value for networks(a-e), respectively.

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Now, to study the details of the effect of symmetry in the efficiency of classical and quantum transport, we study the asymptotic values of $\bar{P}(t)$ and $|\bar{\alpha}(t)|^2$.

Network(b) have eigenvalue 1 with degeneracy 2-fold, (i.e. $D_l = 2$). In Fig. 4(b), after $t \sim 30$, we observe that $\bar{P}(t)$ reaches equipartition 0.1, while $|\bar{\alpha}(t)|^2$ fluctuates about the asymptotic value 0.12. Since the eigenvalue spectrum of network(b) includes eigenvalue 1 with degeneracy 2 and eight non-degenerate eigenvalues, Eq. (14) gives the asymptotic value of $|\bar{\alpha}(t)|^2$ as 0.12 which confirms the numerical result.

In network(c), the degeneracy of eigenvalue 1 is 4-fold and the other eigenvalues are non-degenerate. In Fig. 4(c), we see that at about $t \sim 12s$ the classical curve reaches the equipartition probability 0.1 while the lower bound $|\bar{\alpha}(t)|^2$ fluctuates about the saturation value 0.22, as can be derived from Eq. (14).

Network(d) have eigenvalue 1 with degeneracy 6 and other eigenvalues non-degenerate. In Fig. 4(d), one can see that the classical curve reaches 0.1 at $t \sim 20s$, whereas the lower bound $|\bar{\alpha}(t)|^2$ fluctuates about the asymptotic value 0.4(as can be inferred of Eq. (14)).

Network(e) can well be represented a graph star with 10 nodes whose eigenvalues have three discrete values: eigenvalue 1 with degeneracy 8, non-degenerate eigenvalues 0 and 10 [58]. Fig. 4(e) shows that after $t \sim 8s$, classical probabilities reach 0.1, while not only $|\bar{\alpha}(t)|^2$ but also $|\bar{\pi}(t)|^2$ fluctuate about a constant value 0.66(as can be obtained from Eq. (14)).

We can conclude that, on symmetrical small networks such as those analyzed here, CTRWs can spread faster than their quantum counterparts. Moreover, the classical curves(blue lines) are flattened out and $\bar{P}(t)$ tends towards a limiting value($\frac{1}{N}$) such that with increasing the network symmetry this asymptotic domain is obtained more quickly, which implies a more efficient classical transport, except for networks(c),(d), i.e. however network(d) is more symmetrical than network(c)(D_l of network(d)>D_l of network(c)), the limiting value for it occurs more late.

But with increasing the degree of network symmetry(D_l), the quantum average return probabilities fluctuate about a larger saturation value, which implies a less efficient quantum transport, and there is not any exception among networks(a-e).

The reason of these different behaviors can infer from Eqs. (8,9). Based on Eq. (8), in the classical transport the eigenvalues of the transfer matrix itself dominates the average return probability and the degeneracy of eigenvalues directly dose not play role in increase or decreasing $\bar{P}(t)$, while quantum mechanically(Eq.(9)), the degeneracies of eigenvalues are governing

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$\bar{\pi}(t)$. Therefore, as the above numerical results showed, while the efficiency of classical transport on the mentioned networks has not any exact relation with symmetry, increasing the degree of symmetry decreases the efficiency of quantum transport on them.

5 Conclusions

In summery, we studied CTRWs and CTQWs on some networks with few nodes. We calculated the classical and quantum transition probabilities on the networks and by numerical analysis found that there is high probability to find the walker at the initial node for the CTQW on the mentioned networks due to interference phenomenon, even at long times. Thus, to get information about the transport efficiency, we averaged the quantity of the return probability over the all nodes of network. Then, we studied the efficiency of transport on the mentioned networks by studying the decay rate and the asymptotic value of the average return probability. The numerical results showed that the existence of symmetry in the mentioned networks causes the quantum walks to be less efficient than their classical counterparts. Moreover, we found that the increasing of the symmetry of these networks decreases the efficiency of quantum transport on them.

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